5-Bromovaleric acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C11H17BrO2/c1-3-7-10(4-2)14-11(13)8-5-6-9-12/h10H,4-6,8-9H2,1-2H3
InchiKey: LELREPSXQGXCNR-UHFFFAOYSA-N
Formula: C11H17BrO2
SMILES: CC#CC(CC)OC(=O)CCCCBr
Mol. weight [g/mol]: 261.15

Physical Properties

Property code	Value	Unit	Source
gf	22.50	kJ/mol	Joback Method
hf	-221.82	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.897		Crippen Method
mcvol	182.190	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1601.80		NIST Webbook
tb	602.09	K	Joback Method
tc	810.13	K	Joback Method
tf	436.79	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.77	J/mol×K	602.09	Joback Method
cpg	436.69	J/mol×K	636.76	Joback Method
cpg	449.89	J/mol×K	671.44	Joback Method
cpg	462.40	J/mol×K	706.11	Joback Method
cpg	474.22	J/mol×K	740.78	Joback Method
cpg	485.39	J/mol×K	775.46	Joback Method
cpg	495.91	J/mol×K	810.13	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume